



AHPCCRC Bulletin



Volume 1 Issue 4

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Computational Nano- and Biotechnologies

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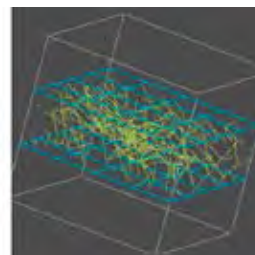
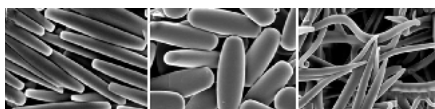
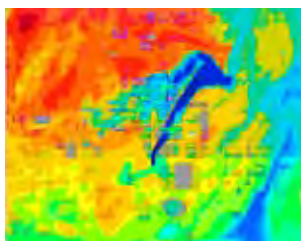
The Army High Performance Computing Research Center, a collaboration between the U.S. Army and a consortium of university and industry partners, develops and applies high performance computing capabilities to address the Army's most difficult scientific and engineering challenges.

AHPCCRC also fosters the education of the next generation of scientists and engineers—including those from racially and economically disadvantaged backgrounds—in the fundamental theories and best practices of simulation-based engineering sciences and high performance computing.

AHPCCRC consortium members are: Stanford University, High Performance Technologies Inc., Morgan State University, New Mexico State University at Las Cruces, the University of Texas at El Paso, and the NASA Ames Research Center.

Material and biological systems at nano- and microscales play an increasing role in Army scientific and engineering endeavors. This research not only draws on existing knowledge of fluid dynamics, molecular modeling, and materials engineering; it requires new insights into the unique behaviors of materials and particles at very small scales. AHPCCRC research in this area addresses two broad classes of problems: detecting, protecting against, and responding to harmful biological agents (natural and engineered); and the rate-dependent response of miniature mechanical components to external loading.

Many important changes happen on the scale of molecules, viruses, and microelectronic devices. Computer simulation is ideally suited to setting up realistic scenarios and studying the interplay of many factors. High performance computing can be used to design strong, lightweight materials “from the atoms up”; to model biological systems at the molecular level; or to simulate the complex interplay of topological and meteorological factors affecting the spread of a contaminant plume. The speed and capacity of massively parallel computers are key to simulating real-world phenomena on scales ranging from nanometers to city neighborhoods. ★



Clockwise from top left: urban aerial visibility map, protein density map and structure model, metal thin film dislocation model, microfluidics test particles, cecropin peptide folding model.

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Dispersion of Biological Warfare Agents in Attack Zones

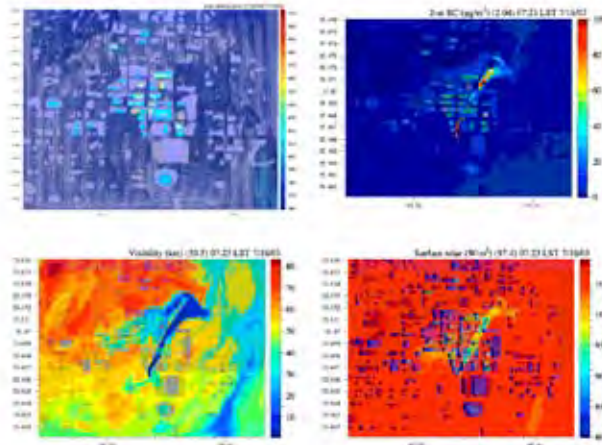
The alert call comes in at the emergency response center. A high concentration of an infectious virus has been detected in the air near a large urban area, possibly as the result of a deliberate hostile act. Which neighborhoods and how many should you evacuate, and how much time do you have? When your organization makes disaster response plans, how will you decide what medical supplies to stockpile and how much?

AHPCRC researchers from Stanford University are tackling these questions using high performance computing to create realistic simulations of hypothetical biological weapon agent (BWA) release scenarios. The team consists of Mark Jacobson (professor of civil and environmental engineering, professor by courtesy of energy resources engineering), Gianluca Iaccarino (assistant professor of mechanical engineering, Institute for Computational Mathematical Engineering), and Eric Shaqfeh (professor, chemical and mechanical engineering, ICME). Gerard Ketefian (postdoc under Jacobson), David Richter (Ph.D. student under Shaqfeh), and David Woodbury (undergraduate student under Iaccarino) also contribute to the research.

The Stanford team is developing a computational framework for modeling the dispersion of particles, from a few nanometers to more than 100 micrometers across, in a turbulent air flow. This computational framework will be used to predict the dispersion of aerosolized BWAs during various indoor or outdoor attack situations. The team has briefed several ARL scientists at the Natick Soldier Systems Center on their results to date. In addition, they have an ongoing interaction with researchers at the U.S. Army Edgewood Chemical and Biological Center and the Army Research Laboratory at Adelphi, Maryland.

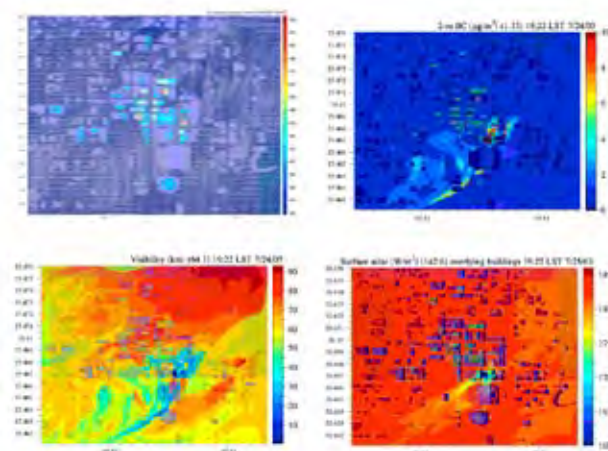
Two Scales

Realistic large-scale or long-term release simulations using engineering models and incorporating motion at all scales is currently outside the reach of even the



Simulations for downtown Oklahoma City, 2003. Above, clockwise from top left: Wind velocity at 2m elevation, black carbon tracer concentration, surface solar radiation, and visibility for 07:23 LST, 16 July. Below: The same parameters for 19:22 LST, 24 July. All graphics courtesy M. Jacobson, G. Iaccarino, Stanford University.

largest available computers. The team is addressing this problem by developing parallel DNS (direct numerical simulation) and LES (large eddy simulation) codes describing the dispersion of rod-like, flexible, or spherical particulate BWAs—including aerosolized organisms or protein toxins—in complex urban environments. Their models will simulate contaminants spreading through volumes of 30–50 cubic meters, about the size of a single room, to begin with. Subsequently, the additional integrated RANS (Reynolds-averaged Navier–Stokes) code will enable complete simulation, including atmospheric interactions, through large-scale spreading over 10–100 square kilometers.



The goal is to perform computations that include the details of the topographic map of the geographic region of interest, while preserving the small-scale motion and mixing in the region of the release. This multi-scale problem is being tackled using two main simulation codes. A large-scale atmospheric code, with resolution ranging from 10–50 m up to a global scale, is used to study the long-time and large-scale evolution of the plume and its interaction with atmospheric agents. A high-fidelity fluid-dynamic dispersion code predicts the dispersion dynamics in the vicinity of the release (0.1–50 m).

The fluid-dynamic dispersion code models the initial dynamics that are strongly affected by the precise release location, concentration, and type of agent, to determine the formation of a release cloud at a scale of 10–25 m. This information is then passed to the large-scale code, which models the evolution of the release over long periods of time. The large-scale code also provides atmospheric boundary conditions (e.g., wind speed and direction, thermal flux) for use in the small-scale code.

The Windy City

The Stanford group began with a model of downtown Chicago, a city that is already well characterized as the result of extensive modeling studies. They analyzed scalar transport and dispersion using their Chicago model and simulated a BWA release for two Chicago locations, in preparation for a grid refinement study to verify the sensitivity of the scalar concentration maps up to 12 minutes after the release.

Although the two release locations in the model were less than 200 m apart, the dispersion patterns are distinctly different (*see figure at right*). In the simulation, high-speed wind channeling along the Chicago River entrained a contaminant plume and caused a fast release in the downstream city blocks. This effect was not observed farther from the river, where closely spaced tall buildings served to disrupt the flow.

The group was able to produce detailed maps of thermal heating (from sunlight) and wind speed and direction using the simulation code.



Simulations for downtown Chicago, 12 minutes after plume release, 30 m above the ground. The two locations are less than 200 m apart, but the plume on the right follows the channel of the Chicago River, while the plume on the left is farther inland.

Within the same computational infrastructure used for the Chicago simulations, the group is developing a model for fluids that do not have one constant value for viscosity, with the intent of representing rodlike and particulate BWAs. The group is modeling the effects of long elastic chains (such as polymers or proteins) in fluids, drawing on a large body of existing literature and computational resources. Their model is now fully functional, and it produces valid results for flow conditions that are more laminar than turbulent. Future work will test the limits of the range of turbulence and shear conditions for which the model is valid. The group will also incorporate nonhomogeneous concentration effects into the model.

Real-World Data from Oklahoma City

More recent simulations (*see figures, page 2*) focus on downtown Oklahoma City, the site of the July 2003 Joint Urban Atmospheric Dispersion Study (<http://ju2003.pnl.gov>). This study, cosponsored by the U.S. Department of Energy, Department of Homeland Security, and the Department of Defense's Defense Threat Reduction Agency (DTRA), featured ten releases of nontoxic sulfur hexafluoride gas and three types of nontoxic perfluorocarbon tracer gases in and around Oklahoma City buildings. This was the largest-ever U.S. urban atmospheric study, involving 150 scientists, engineers, and student assistants, 200 wind measurement stations, and 200 sampling stations.

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Dispersion of BWAs in Attack Zones

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The Stanford group's 20-minute numerical simulations (*box, below*) showed that the direction and intensity of the wind have a profound effect on the flow characteristic in the region of the release. The calculations tracked the spread of a simulated black carbon tracer, under conditions replicating those for the real-world study. The simulated tracer was released at the same location for both simulations, under early-morning and late-afternoon conditions, with the wind shifting to the opposite direction from one simulation to the next. The simulations demonstrated the influence of the tracer plume on visibility and surface solar radiation.

Wind field data from the large-scale model was used to initialize the high-resolution computational fluid dynamics model.

The group continues to validate their computational tools using the Oklahoma City data. They intend to demonstrate the applicability of both the large-scale atmospheric code and the high-fidelity small-scale tool as applied to this problem, and to develop the capability to transfer information between the two codes to accurately predict both the detailed initial release and the long-term behavior of the agent release.

Studying the Wake

In a second area of this project, the research group has performed a detailed study of the dispersion effects downstream of an elongated obstacle, such as a building. This area of work will support the small-scale,

Oklahoma City Simulations

The Stanford team ran two simulations for virtual black carbon tracer plumes emitted from the same downtown Oklahoma City location. One simulation replicated the conditions for July 16, 2003 at 07:00 LST and the other for July 25, 2003 at 17:00 LST. The wind blew in opposite directions on these two days. (LST, local sidereal time, denotes the position of the sun in the sky rather than the local time zone.)

The simulations were done on four size scales: global (4 degrees latitude \times 5 degrees longitude resolution), U.S. (about 50 km resolution), Oklahoma (120 m S-N \times 120 m W-E \times 20 m vertical resolution), and Oklahoma City (12 m S-N \times 12 m W-E \times 20 m vertical resolution).



Two-dimensional simulation of turbulent flow in the wake of a building.

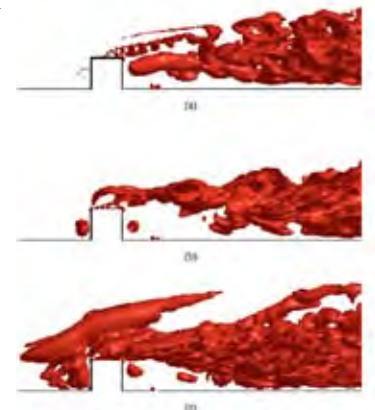
high-resolution calculations that predict flows around and over objects of arbitrary shape (e.g., buildings).

In this case, the high-fidelity code is used with highly refined grids, and the results are compared to existing detailed experimental measurements. The numerical simulation agrees exceptionally well with the mean flow measurements, the turbulent fluctuations, and the transported scalar statistics.

Additional simulations using low-fidelity Reynolds-averaged models illustrate the limited predictive capabilities of these schemes. The predictions for scalar and recirculation bubble concentrations, vary significantly, depending on the type of model used.

At present, the Stanford group is completing an investigation of the detailed dispersion downstream of the obstacle to identify the importance of large-scale three-dimensional effects (*see figure below*).

In addition to the simulations, the Stanford team is developing a new computation flow code that will be the first to conserve a combination of properties, including potential enstrophy, vorticity, energy, and mass, when arbitrary boundaries are treated. This capability facilitates model-building by specifying which aspects of a system change and which remain constant. ★



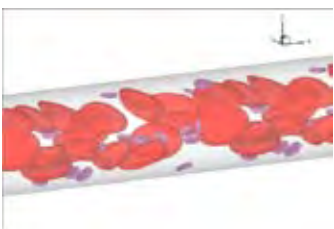
3D turbulent flow simulations. Top: inflow fluctuations ignored. Middle: random inflow fluctuations imposed. Bottom: force with most unstable modes.

Micro-and Nanofluidic Simulations for BWA Sensing and Blood Additive Development

Microfluidics is the study of suspensions and solutions flowing through channels barely large enough for particles to pass. Microfluidic models provide valuable insights on designing portable devices for sensing and identifying biological warfare agents (BWAs), as well as for developing medical treatments for traumatic injuries. Many lab-on-a-chip devices contain fluid channels just wide enough to accommodate a few large molecules such as DNA. Some molecular “bar code” devices contain capillaries that force submicron objects to pass through a channel in single file. Human capillaries can be narrower than a single red blood cell, forcing cells to deform in order to squeeze through.

When the width of a channel is roughly the same size as the particles flowing through it, conventional fluid dynamics principles no longer apply. Essentially all of the particles are in contact with the walls of the channel, leaving no area of free flow in the center. Particle shapes and channel dimensions and geometry take on increasing importance. Irregularly-shaped or elongated particles can form snags and obstructions, like logjams in a stream. Particles adhering to the channel walls (blood clots, for instance) affect the characteristics of the flow. If the particles interact electrostatically with the channel walls or with each other, this adds additional complexity.

Eric Shaqfeh (professor of chemical and mechanical engineering) and Eric Darve (assistant professor of mechanical engineering) are members of Stanford University’s Institute for Computational and Mathematical Engineering. Their work for AHPCRC



expands existing modeling and simulation capabilities

Red blood cells (red) and platelets (blue) in a blood vessel.

to construct methods that realistically reproduce and predict the behavior of particles in a microfluidic stream under a wide variety of novel conditions. Their models take into account factors such as electrical forces, flexible or rigid particles of various shapes, Brownian (random) motion, and sedimentation effects.

At present, no computational simulation techniques exist that include all of these factors in the same package. The simulation codes under development by Shaqfeh and Darve handle orientable objects in a flow with hydrodynamic interactions. They are adding and integrating capabilities for complex microfluidic environments and particle shapes, deformable particle surfaces, complex interactions between the solid and liquid phases, and adhesion effects. Other factors in the model include electrical charge effects, mean flow, channel wall interactions, and sedimentation.



Rod-shaped particles in microfluidic channels. All graphics courtesy of Eric Shaqfeh, Stanford University.

Sensing Devices

Electrostatic interactions, channel geometries, and wall adhesion effects can be put to use in sorting and sensing various types of particles, including proteins and viruses. Indeed, several compact field testing devices on the market now use microfluidic channels to detect and identify substances of interest, using length, shape, electrical charge, and chemical affinities as identifying characteristics.

Numerical simulations of particles in microchannels imitate their real-life counterparts—the virtual particles start at a simulated inlet well and are driven electrokinetically through a simulated channel, where they are separated by size or electrical charge, adhere

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Microfluidic Simulations

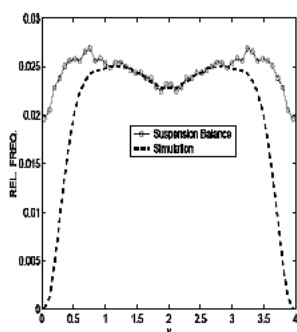
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to the walls according to predetermined interaction potentials, or separate into different channels. In the laboratory, real particles would be sent to a sensing area where various analytical devices could identify them and determine their concentrations. In a simulation environment, numerical methods are used to perform tracking and measuring functions. The success of the simulation method is determined by how well it emulates laboratory observations for known systems, and how useful it is for predicting the behavior of new systems.

All relevant interactions among the particulates and with the micro-device walls must be included in a simulation in order to produce realistic predictions of particle behavior. Particles can separate or form aggregates with each other. Layers of particles can build up on the channel walls. In addition to electrokinetic forces, shear, drag, and Brownian motion influence the overall flow.

Capabilities already exist for simulating sedimentation and Brownian motion for rod-like particles and semi-flexible molecules such as DNA. Under the AHPCRC program, Shaqfeh and Darve have completed their computer code for planar channel flow simulations, and this code is being benchmarked and adapted to parallel computing environments. The existing models account for hydrodynamic interactions and the volume excluded by the particles, and the models can use electro-osmosis or pressure as the driving force.

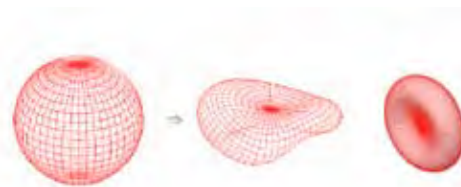
The AHPCRC group has used their models to predict



nonuniform concentration profiles across small channels as a result of variations in osmotic pressure. They are

Concentration profile showing more particles near the channel walls. Solid line: observed; dotted line: simulation.

Spherical harmonic model of a cell surface (left and center), red blood cell model (right).



determining whether this effect can directly separate particles based on length by comparing their simulations with microfluidic experiments conducted by Dr. Samir Mitragotri, an associate professor of chemical engineering at the University of California at Santa Barbara who is an active member of the Institute for Collaborative Biotechnologies (ICB).

The simulation capabilities are being expanded to include complex particle shapes and channel geometries. Dynamic simulations are in progress for nano-channel separations of short double-stranded DNA (up to 100 base pairs). The simulations include center-of-mass and rotational Brownian motion, molecular interaction with the electronic double layer potential (a type of wall interaction effect), and electro-osmotic convection. Scalable algorithm development for the calculations of the long-range interactions (electric and hydrodynamic) is essential in these simulations. The AHPCRC group is focusing on comparison of these simulations with the experimental measurements and modifying them for flow through more complex microfluidic geometries, including multiple channels, T-junctions, and bifurcations (forks in the channel).

Blood circulation

Blood vessels may be thought of as microfluidic channels, and studies of particles in small channels may be applied to the movements of particles in the bloodstream. Such particles include cells, blood additives (oxygen carriers and reconstituted or artificial platelets), particulate (non-dissolved) drugs, and drug delivery agents. Particles may be spherical or rod-shaped, rigid or flexible, and electrically charged or neutral. Particles may be driven through the channels using pressure (e.g., heartbeats). An electric field or electrostatic charges may drive the motion of the particles (electrophoresis) or the surrounding fluid

(electro-osmosis), a set of processes known collectively as electrokinesis.

Army medical researchers are especially interested in developing methods for processing human blood platelets so that they can be freeze-dried for storing and shipping, then reconstituted in the field for the treatment of serious wounds (see “*The Push for Platelets*,” below). Current techniques for lyophilization (freeze-drying) require a multi-step procedure involving chemical fixers to keep the platelets from agglom-

erating, and reconstituted platelets are not as effective as platelets in their native state. Despite these factors, lyophilization offers significant advantages in remote field clinics. Recently, the Stanford group completed its first computer simulations of platelet and red blood cell microcirculation behaviors. These simulations show that, at the high shear rates typical for small vessels, red blood cells gradually move toward the center of the blood vessel, forcing the platelets toward the vessel walls, in good agreement with experimental observations. ★

The Push for Platelets

Donated blood is the most common treatment for acute blood loss arising from invasive surgery or traumatic wounding. Donated whole blood can be stored for approximately one month under the proper conditions. Recipient blood types must be cross-matched against available stocks of donor blood, and the threat of spreading infectious diseases such as HIV and hepatitis cannot be eliminated completely. These limitations are exacerbated in field situations, where electricity for refrigeration may be sporadic and a supply of suitable donors is limited. Donor blood can be used more efficiently by separating it into components—including platelets—that are processed for storage and transport. Fresh platelets must be used within five days of donation, and laboratory testing may require as much as one day.

Platelets act as “first responders” at a wound site. Damage to blood vessel walls exposes collagen structural material to direct contact with the bloodstream, activating the platelets and causing them to release granular particles containing tissue growth factors. The growth factors attract fibrin from the blood plasma, which forms a mesh that stops blood loss. Other growth factors stimulate the formation of new tissue cells on the fibrin scaffolding.

Platelets can be stored for clinical use by treating them with preserving agents such as glycerol or dimethyl sulfoxide (DMSO) to prevent agglomeration, then freeze-drying them (lyophilization). The platelets are thawed and rehydrated at the time of

use, which can be up to several months after donation. Reconstituted platelets must be washed and processed to remove the preserving agents, which requires specialized equipment and generates by-products that must be disposed of properly.

Many platelets are damaged or destroyed during reconstitution. Reconstituted platelets often have a balloon shape that not only affects their ability to circulate in the bloodstream, but makes them unresponsive to biochemical stimulants (agonists, such as thrombin) that would normally activate the clot-forming behavior of the platelets. Reconstituted platelets are less than 35% as responsive to wound-generated agonists as fresh platelets.

Wound treatments derived from platelet-enriched concentrates offer the benefits of platelet-generated growth factors and wound sealing properties that stop blood loss. However, the concentrate must be applied to the wound site within a few seconds after the activating agent is added, because hardening is almost instantaneous. The concentrates are often derived from the patient’s own blood, and they must be re-applied daily. This requires repeated blood withdrawal from the patient and on-site processing procedures.

Lyophilized platelet treatments avoid problems associated with platelet concentrates, and thus, are of great interest to Army medical researchers.

Reference: U.S. Patent application 20080213238, James Bennie Gandy and Mackie J. Walker

Antimicrobial Peptides for Nanoengineered Active Coatings

Antimicrobial paints and fabric treatments offer a lightweight, economical, form of personnel protection against biowarfare agents (BWAs) and other pathogens. These coatings also protect vehicles and equipment from the corrosive effects of microbial secretions, and antimicrobials retard the spoilage of latex paints.

In 2007, the U.S. Army reported annual expenditures of more than \$100 million for topcoat materials to protect against chemical agents. Several coating methods, such as chemical vapor deposition, are effective for small surfaces but are not practical for large equipment or vehicle coatings. Newer technologies, such as self assembled monolayers, do not hold up well in harsh environments. Effective coatings must adhere well without compromising or damaging the surfaces to which they are applied.

Recent research has focused on peptides, the molecular building blocks of proteins, as components of antimicrobial paints and coatings (*see figure, page 9*). Antimicrobial peptides, which are common in nature, protect the underlying organism or structure by disrupting the cell membranes of bacteria that come into contact with the coating (*see figures at right*). Antimicrobial peptides act by forming large holes in cell membranes or by carpeting membrane surfaces in a manner similar to detergents.

Eric Darve, assistant professor of mechanical engineering at Stanford University, is developing high performance computer simulation capabilities to further the understanding of the molecular mechanisms behind this antimicrobial activity, as the focus of a project for AHPCRC that began in early 2009. His simulations will also prove useful in identifying and designing peptide mutations that work well in polymer coatings being developed by the Army.

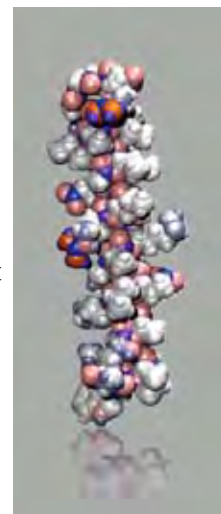
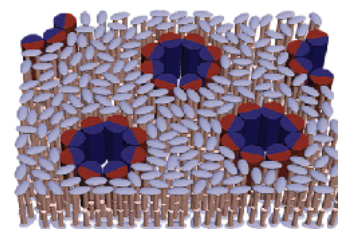
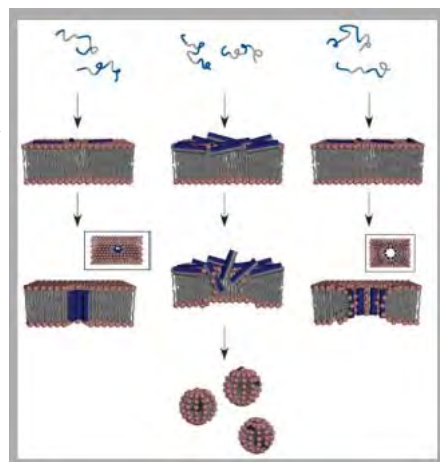
Darve is working in tandem with Jan Andzelm and Lars Piehler, researchers at the Army Research Labo-

ratory's Weapons and Materials Research Directorate at Aberdeen Proving Ground, Maryland (WMRD APG), who are producing experimental data in their laboratories.

Improving on Nature

Darve and his Army collaborators are especially interested in a well-characterized group of peptides called cecropins. These peptides were originally isolated in the early 1980s from the giant silk moth, *Hyalophora cecropia*, but their molecular relatives are found in many species of winged insects. As you might expect, cecropins protect their insect hosts against invasive micro-organisms. They do this by attaching themselves to and opening large pores in microbial cell membranes.

By varying the amino acids that form the cecropin peptide, analogs have been produced that are more potent than the parent compounds. This indicates that intentionally-designed cecropin analogs could be produced for specific applications and conditions. In order to do this, however, the mechanisms by which these peptides do their work must



Top: Protein molecules are attracted electrostatically to the bacterial cell membrane.

Middle: Hydrophobic sections of the protein penetrate and breach the membrane.

Bottom: Structure of an antimicrobial protein molecule.

(Top and bottom images, Eric Darve; middle image, Oak Ridge National Laboratory)

be understood much better than they are at present. Computer simulations are ideally suited for this type of exploratory work, in that a large number of alternatives may be explored, and patterns may be identified that point the way toward the most promising candidates.

Any useful synthetic peptide must preserve cecropin's ability to distinguish between negatively-charged bacterial (prokaryotic) cell membranes and human or animal (eukaryotic) cell membranes, which have positively and negatively charged regions. Peptide molecules are made from electrically charged (hydrophilic) and electrically neutral (hydrophobic) sections. These complex molecules fold and unfold, depending on their thermal and chemical environments. The portions of the folded molecules, charged or uncharged, that face outward determine whether the molecule is attracted to and adheres to a particular type of cell membrane. Laboratory work has shown that helical molecules having a net positive charge are the most active forms for binding to the negatively-charged exteriors of bacterial cells. Once the molecules attach themselves to a bacterial cell membrane, a mechanism must be found for making the hydrophobic sections of the helices available to penetrate and breach the membrane.

Simulation work

Computer resource requirements are the greatest limiting factor in the simulation of such biomolecular systems. Simulations of this sort must model such molecular behaviors as helix formation, unwinding, insertion into a membrane, and self-assembly over relatively long time scales—microseconds to milliseconds. Current software and numerical methods do not allow modeling over the necessary time scales; Darve places a high priority on creating algorithms that would enable this gap to be bridged.

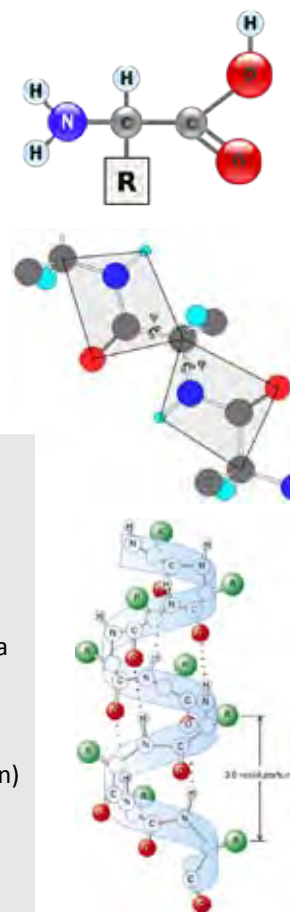
Darve's main software platform is NAMD, a large-scale parallel code for molecular dynamics simulation of proteins and cell membranes. This code is robust and faster on parallel computers than most competing codes. At present, the NAMD computer code can simulate 6–22 nanoseconds of molecular behavior per

day of execution time, using 128 processors in parallel (38,000 atoms, 2 femtosecond time step).

Darve has determined the structure of cecropin in water and at a polar–nonpolar interface (such as the interface between water and a cell membrane). These molecular simulations made it possible to validate the force field parameters. He has found that the molecule starts to unwind when the protein is in bulk water, which is consistent with experimental findings.

Future Work

For the immediate future, work will center on the basic science aspects of the molecular models: validating the molecular force fields used in the model and investigating the behavior of cecropin in water and at nonpolar interfaces. These studies will provide a foundation for models of the interactions between cecropin and various types of cell membranes. Darve has developed some novel techniques to analyze long time-scale events, and these will be used to determine the unfolding and folding mechanisms. Later studies will evaluate the antimicrobial properties of cecropin and its variants to identify the most promising candidates for inclusion in active coatings. During the course of this research, the results will be validated against experimental work done at ARL. ★



Top: Amino acid. R is a generic hydrocarbon group—a hydrophobic residue. Nitrogen (blue) and oxygen (red) form the hydrophilic residues. Middle: Amino acids link to form a peptide chain. Bottom: Peptide chains link to form a protein molecule. (Top image: Wikimedia Commons, middle and bottom images: National Center for Biotechnology Information)

For more information on protein structures, see “How to Build a Virus (Structure)” on page 11.

Protein Structure Prediction for Virus Particles

Maintaining troops in a ready state requires that they be in good health. Lethal viruses pose an obvious threat to readiness, but even a rampant infestation of the sniffles can keep a battalion from operating at its best. Effective vaccines against viral infections—naturally occurring or introduced by hostile forces—are a moving target. What worked on last year's virus may be ineffective on this year's mutated strain, a completely new virus, or a genetically engineered or weaponized virus.

The U.S. Army has been active in the development of vaccines against the viruses that cause malaria (*Plasmodium vivax*); diarrheal diseases (e.g., *Rotavirus*); dengue fever and yellow fever (flaviviruses); and spotted fever and typhus (*Rickettsia*). The Army is also actively pursuing research on highly lethal viruses, including those that cause hemorrhagic fever.

Understanding the mechanisms by which viral diseases originate and develop requires a knowledge of the three-dimensional structures of the proteins that make up disease-causing viruses, says Jing He, assistant professor of computer science at New Mexico State University. (Prof. He recently accepted a faculty position at Old Dominion University.)

Under the AHPCRC program, Prof. He, her graduate students Kamal Al Nasr and Saeed Al-Haj, and postdoctoral fellow Weitao Sun are developing a scalable parallel computer code for identifying the most likely viral protein structures from a very large set of possible topologies. They are working from the ground up, a technique called *ab initio* prediction. The “ground” in this case is a set of low-resolution protein electron density maps. This information can be generated using biophysical laboratory techniques such as electron cryomicroscopy, and density maps are readily available in the literature. The resolution of such maps is typically 5–10 Å, or about 3–8 carbon atoms across. The challenge is to take a primary structure (a known sequence of amino acids), and map it onto its

corresponding secondary structures. These secondary structures—the helices and sheets formed by the amino acids—can be visualized using the density map. (See “How to Build a Virus (Structure)”.

Like fuzzy photographs, these low-resolution density maps delineate the general outlines of a protein's shape, but the outline is often incomplete and only displays the regions where the atoms are densely populated. He's group is working to “sharpen” these images. Ultimately, they hope to derive the spatial coordinates of the individual atoms that are included in the protein, using geometrical constraints to sort out the most likely topologies.

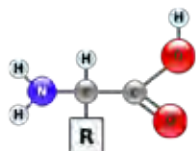
To derive the spatial coordinates of the atoms, a coarse-level mapping must be derived between the amino acid sequence and the secondary structures in the density map. Such a mapping determines the possible topologies of the secondary structures of the density map. Then the coordinates of the atoms can be constructed using the likely topologies. The literature contains detailed experimental studies of the atom-by-atom structures of existing proteins, and this provides information on the energies (and thus, the relative stabilities) associated with various topologies.

Testing the Concept

He selected 51 well-characterized proteins at random from the Protein Data Bank, a central repository of known protein structures. The selected proteins were required to have one single domain (i.e., no part of the protein could be capable of evolving or functioning independently of the rest of the protein), and the structure must have been determined to a resolution of 1.5 Å or better (to the level of individual carbon atoms). None of the proteins had a more than 30% similarity in their amino acid sequences, and each protein had fewer than 8 secondary structures (because of constraints on computing resources). All possible secondary-structure topologies were generated computationally for each of the 51 proteins, and the conformational energies for each topology were calculated using a multi-well Lennard-Jones potential function.

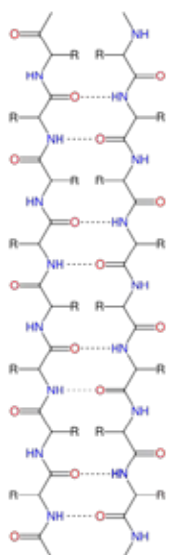
continued on page 12

1)



How to Build a Virus (Structure)

2)



Starting from chemistry

1) Amino acid molecules (like the one shown here) link in specific sequences, or primary structures, to form protein chains. (R is a generic hydrocarbon chain.)

2) A beta sheet containing two hydrogen-bonded protein strands.

3) Protein chains can also coil into alpha helices (shown here as a secondary-structure representation of myoglobin).

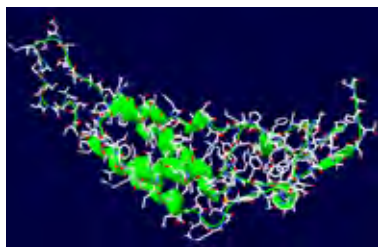
4) Crystallographic studies resolve secondary structures into tertiary structures—3D arrays of atomic coordinates (shown here: tobacco mosaic virus).

5) Protein molecules cluster together to form quaternary structures (human hemoglobin shown here, protein subunits in red and blue).

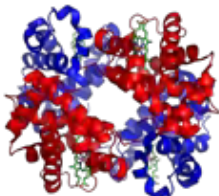
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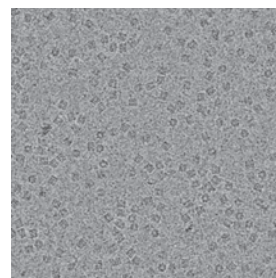


5)



Starting from microscopy

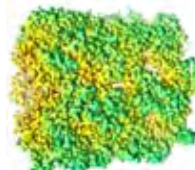
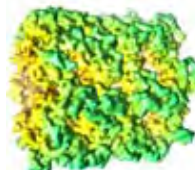
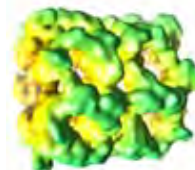
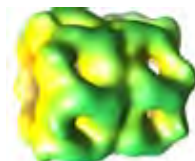
6)



6) Electron cryo-micrograph of GroEL (suspended in vitreous water ice), a chaperone protein complex that assists newly formed bacterial protein chains to fold into a functional 3D form.

7) Electron density maps for GroEL. Resolutions in Ångstroms from top to bottom: 32, 16, 8, 4.

7)



8) Density map (light gray) is used to construct geometric constraints that indicate the most likely configurations of protein structures. (Protein 1A0P shown in 8 and 9. Red: predicted structure, dark gray: native structure)

9) To predict the structure from the density map, a large number of conformations are sampled, using the amino acid sequence of the protein to construct the backbone and the sidechains of the protein.

8)



9)



In real life

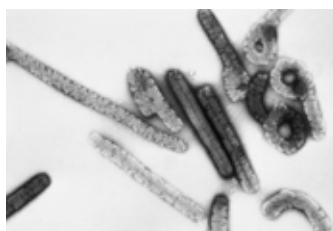
10) Particles of the Marburg virus, which causes a type of hemorrhagic fever.

1–7: Wikipedia (public domain and GNU Free Documentation License).

8–9: Jing He, NMSU.

10: U.S. Centers for Disease Control.

10)



Protein Structure Prediction for Virus Particles

continued from page 10

He's group uses geometrical constraints to evaluate the energies required by various protein topologies, to find the most "comfortable" configurations of bends and folds assumed by the protein's helices, sheets, and strands. The method is being developed using known structures of naturally occurring proteins, and the assumption is that the order and directionality of the secondary structures that these proteins assume under natural conditions—the native topologies—are the most stable (requiring the least energy). If the computer model can reliably identify the native topologies in their set of most-stable structures, this builds confidence in the model's ability to predict structures of newly encountered or engineered proteins.

In most cases, the calculations placed the native topology among the most stable of the possible topologies. Of the 48 possible permutations of protein IDV5, two conformations (4% of the total 48) were more stable than the native topology. The native topology of IQC7, with 46080 possible topologies, was more stable than all but 14 possible conformations (0.03%).

But Does It Scale?

Because of the flexibility and complexity of protein chains, considerable computing resources are needed to evaluate and compare the relative energies associated with the numerous possible combinations of structural features. As might be expected, this sort of calculation requires significant computational resources and a program for visualizing the resulting three-dimensional structures. Every algorithm developed under this project requires implementation in parallel code to collect necessary data.

As a part of this study, two parallel computing strategies were employed. In the static work allocation scheme, the possible permutations for a given protein structure were distributed evenly among all available processors. Each processor "knew" what its sequence of tasks would be, and when it finished a given task, it would automatically start on the next one. This strategy minimizes communication between processors,

but processors assigned to faster tasks may sit idle as the other processors complete slower tasks. The second strategy was a dynamic scheme, incorporating a master processor that assigned new tasks, or pieces of tasks, when the "worker" processors signaled that they had completed the previous task.

When fewer than 32 processors were used, the static work allocation completed the calculations more rapidly for all but the two smallest proteins, because all the processors contributed to performing the calculations. The dynamic model, which requires one master processor that allocates tasks, but does not participate in the calculations, exhibits a comparative advantage when more than 32 processors are used. For 32 processors, the dynamic method was up to 31 times faster than the static method. A load balancing method, currently under development, distributes jobs to the individual processors. The research group is investigating an affinity method that uses a message passing interface to control the work that is sent to the preferred processors.

Current and Future Work

In the early stages of this project, much of the effort was devoted to finding a way to establish an effective energy function—an important factor in structure prediction, since trial structures having the lowest overall energy are presumed to be the most stable, and thus the most likely to occur. Currently, the researchers are trying to develop a more accurate estimation of the energy by incorporating the geometrical orientations for the protein sidechains.

The program is also being modified to handle larger protein molecules. A parallel simulated annealing optimization scheme has been incorporated in place of the previous enumeration scheme. The simulated annealing method is well suited to finding an acceptably good solution, such as a small subset of likely structures within a large number of possible permutations, rather than one best solution, which the enumeration process tries to find. This modification is currently being evaluated for its ability to predict large protein structures. ★

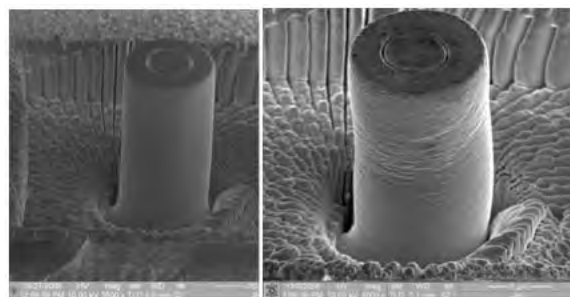
Nanomechanics of Metal Plasticity of Thin Films and Cylinders

Just as small-scale flying machines and microfluidic channels behave far differently than their large-scale counterparts, microscopic mechanical parts and metal films present unique design challenges not observed at a larger scale. Properties such as particle size, microstructural features, and film thickness take on a greater importance with respect to mechanical properties, impact resistance (or impact effectiveness), behavior under stress, and modes of failure. Thus, microscopic devices cannot be designed simply by scaling down their macroscale counterparts, even if they are made from the same materials.

Material properties, including yield stress and defect propagation, at or below the micron scale (0.001 mm; a human hair is about 25 microns across) are not well understood, especially under rapid deformation and high strain rates, where experimental data is difficult to obtain. Particle sizes and surfaces play a greater role in components that are on the same size scale as individual grains. High-performance computer modeling and simulation offer capabilities for predicting and understanding such behaviors, which in turn, can guide the rational design of new materials and configurations.

Wei Cai, assistant professor of mechanical engineering at Stanford University, is working with research associate Sylvie Aubry and graduate students Christopher Weinberger and Jie Yin to develop metal microstructure modeling capabilities under the AHPCRC program. Their research follows two main directions: the response of metal micropillars under tensile and compressive deformation, and thin metal films that undergo tensile or cyclic (fatigue) loading conditions.

Cai and his group are developing modeling capabilities using a method called dislocation dynamics (DD), which tracks defect motion through a crystal lattice. They are comparing their results with those obtained using molecular dynamics (MD) modeling, which characterizes the behavior of atoms and small ensem-



Scanning electron micrographs of nanocrystal BCC tantalum micro-pillars (about 5 microns diameter) before and after a compression test. Courtesy Qiuming WEI, University of North Carolina at Charlotte, Department of Mechanical Engineering, in collaboration with ARL's Brian Schuster.

bles of atoms, with the intent of bridging these two methods and the length scales to which they apply.

Shear Banding

Impact studies on metal parts, including vehicle panels and projectile tips, have turned up a microscale phenomenon called adiabatic shear banding (ASB). This, in turn, has provided important insights into why metallic parts bend and break. Shear bands act as sites for future failures. Voids and other defects appear in the shear bands after a shock event, as the material recovers in its deformed state.

Shear bands form in metal when the stress and deformation are localized into a small area. "Adiabatic" refers to the absence of heat transfer: strain rates are so high that there is not enough time for the heat to diffuse away from the deforming zone, causing a local softening of the metal. Formation of ASBs helps the tip of a projectile tip penetrator stay sharp during impact, because thin layers of metal shear off as the projectile penetrates the target. Shear bands are a detrimental feature for armor parts or machine parts that experience repeated shocks (forging, impact, electromagnetic forming, etc).

ARL-sponsored research found that ASBs form in certain body-centered-cubic (BCC) metals when their grain size is below 1 micron (See "Anatomy of a Dislocation," page 16). FCC metals do not exhibit this property. The origin of this size effect is still under debate.

continued on page 14

Nanomechanics of Metals

continued from page 13

Researchers Brian Schuster and Reuben Kraft (ARL Weapons and Materials Research Directorate) want to understand the mechanical properties of BCC metal nanocrystals, in order to design better armor materials. As a way to characterize these materials, they perform compression and tensile tests on micro-pillars cut from BCC metal nanocrystals. They are searching for material systems that combine high strength, the ASB mechanism, and tensile ductility. They are studying the effect of the grain boundaries on mechanical strength, and they have observed that fine-grained metals experience more ASB than do more coarse-grained metals.

Cai's group is doing dislocation dynamics simulations for micro-pillars made of single crystals. Both research groups are coordinating their studies on micro-pillar deformation, so that the computer simulations and experimental measurements can be compared to each other.

MEMS Actuators

Microelectromechanical systems (MEMS)—tiny machines made of sensors and actuators a few microns in size—have been finding increased application as switching devices, components in consumer electronics devices, miniature sensors, and telecommunications equipment. Because of the small size of MEMS devices, electrostatic and surface effects take precedence over such macroscale properties as inertia

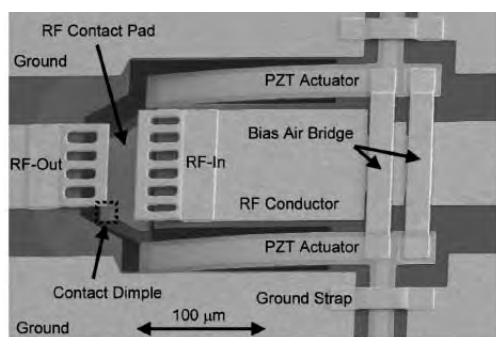
or thermal mass. MEMS devices can be manufactured using technologies similar to those used for computer chips. Multiple thin-film layers are deposited on a rigid substrate, then etched or micromachined into gears, cantilevers, and channels.

Dr. Madan Dubey's group at ARL is developing a multilayer MEMS that uses thin films of PZT (lead zirconium titanate, a piezoelectric material) as the actuating material and platinum metal as the electrode. The thickness of the platinum film layers determines how many actuation (bend-and-release) cycles they can undergo before an accumulation of dislocation defects causes metal fatigue and failure. Understanding dislocation dynamics in metal and semiconductor thin films is important for ensuring the reliability of these novel MEMS and electronic devices.

Modeling Tools

Micro-compression experiments on individual pillars have shown that the amount of stress necessary to sustain plastic deformation increases dramatically from the bulk value once the pillar diameter drops below one micron. That is, it takes more force applied to a given cross-sectional area to induce plastic deformation of a micro-pillar than for a macroscopic pillar. This is a size effect that is beyond the scope of conventional plasticity theory and constitutive models (which describe the response of a material to external forces). The physical basis for this effect is not well understood, but it is widely accepted that explicit large-scale defect dynamics simulations are more faithful to the underlying physics, provided that the computer program is able to handle a sufficient number of defects for a long enough time.

The main challenge in predicting materials strength by computation lies in the gap, roughly 10^{-9} to 10^{-3} m, between the fundamental physics of atoms and phenomenological models of a continuum. To this end, the dislocation dynamics (DD) simulation method was invented, with the goal of directly computing the plastic strength of crystals in terms of the motion of their dislocations. This vision has not yet been realized because of the tremendous number of dislocation seg-



Multilayer MEMS device with piezoelectric lead zirconium titanate (PZT) actuators coated above and below with thin platinum films. Micrograph courtesy Dr. Madan Dubey, ARL.

ments that must be included in a statistically meaningful simulation.

The main challenge in applying DD simulation to metal micro-samples is the need to account for the image stress produced by the free surfaces. Existing DD simulations in micropillars and thin films do not have an efficient image stress solver and do not scale well on large number of processors.

Cai and his co-workers at Lawrence Livermore National Laboratory have developed a publicly available, massively parallel dislocation dynamics simulator called ParaDiS (Parallel Dislocation Simulator, <http://paradis.stanford.edu>), with the intention of overcoming many of the problems associated with conventional dislocation dynamics programs. By using thousands of processors simultaneously, ParaDiS has, for the first time, successfully captured the strain hardening behavior of a $10\mu\text{m}^3$ representative volume in a bulk metal. It runs routinely on 100–1000 processors, including Stanford's local cluster SU-AHPCRC and the Navy DSRC Cray XT5 EINSTEIN. The scalability of ParaDiS has been demonstrated on the 132,000 processors of the BlueGene/L supercomputer. Thus, ParaDiS can take advantage of more parallel computing power as it becomes more readily available in the near future.

Under the AHPCRC program, Cai is developing numerical algorithms and computer programs (implemented in ParaDiS) that allows DD simulation of thin films and micro-cylinders. An efficient image stress

algorithm has been implemented in ParaDiS for thin film and cylinder geometries. The thin film algorithm is also working in parallel.

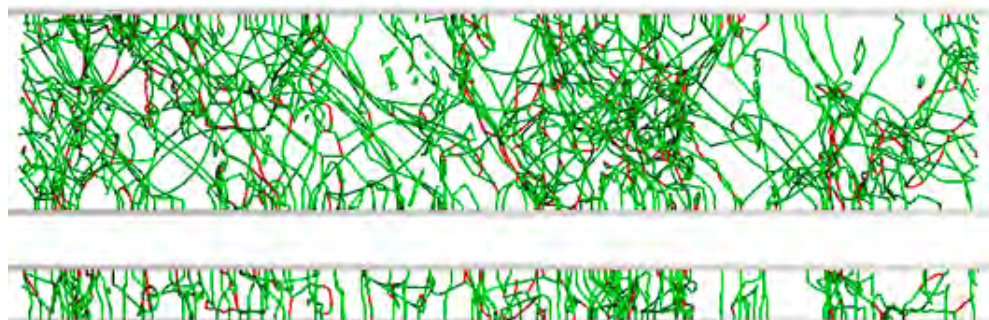
Cai is conducting a quantitative comparison between DD and MD simulations of dislocation behavior in thin films and micro-cylinders. The DD and MD predictions on dislocation equilibrium angles in thin films agree well with each other. DD and MD predictions also converge on dislocation behavior (self-multiplication) in micro-cylinders.

Future work

Efforts are underway to understand the size effect in plasticity of thin films and micro-pillars undergoing uniaxial loading and bending, using large-scale DD and MD simulations. Dislocation–grain boundary interactions are being incorporated into the DD model, assisted by insights from MD simulations. Another observation from MD simulations, the kink pair mechanism of dislocation motion in BCC metals, will also be incorporated into DD. A quantitative comparison between DD and MD simulation predictions and laboratory micro-tensile tests of single-crystal and bicrystal BCC pillars is planned for the coming year.

ARL scientists are constructing a lab setup for tensile and compression tests of micron-sized metal pillars to enable direct comparison between model predictions and experiments. ★

Dislocation models for metal films under tension. Top: thicker film has dislocations in many directions. Bottom: dislocations are preferentially aligned in a thinner film. ParaDiS simulation courtesy Dr. Wei Cai, Stanford University.



Anatomy of a Dislocation

Metallic elements and alloys exist as crystalline materials: orderly three-dimensional arrays of atoms that form small particles called grains. Metallic grains adhere to one another to form the macroscale structures we recognize as paper clips, coins, gears, and sheet metal. Thin metal films and microscopic metal devices are only a few grains across, and they behave very differently from their larger counterparts.

Metals differ from other crystalline materials such as ceramics or gemstones in their ability to deform—bend, flatten, or be drawn into wires—without breaking. Planes of metal atoms glide past each other like layers of ball bearings and settle into new positions that maintain the overall integrity of the crystal structure.

This process is not perfect, however. Each time a piece of metal bends, planes of atoms slip past each other. In the process, some of these planes become misaligned to form structures called dislocations. Dislocations can travel through the structure, and when enough of them accumulate, a crack forms. In thin metal films, the distance from the interior to the surface is small, so the interaction of dislocations with the surface becomes a driving factor. Dislocations that reach the surface of the metal disappear, or “exit,” but can leave behind various types of structural imperfections, depending on the metal’s crystal lattice structure.

Two common structures for metallic crystals are body-centered cubic (BCC) and face-centered cubic (FCC). Metals with a BCC structure, including tungsten, chromium, and molybdenum, tend to be strong and moderately ductile. Soft, ductile metals such as aluminum, copper, nickel, and platinum assume an FCC configuration. (Brittle metals such as zinc, titanium, and magnesium take on a third structure, not addressed under the current AHPARC project, known as hexagonal close packing.)



A moving dislocation (pinned at both ends) encounters an immobile dislocation near its glide plane. The moving dislocation cross-slips to a different glide plane to bypass the obstacle. Image courtesy Dr. Wei Cai, Stanford University.

Metal micropillars are convenient stand-ins for macroscale test bars when the compression tests are performed at a very small scale. “Forests” of micropillars can be grown and cut from a thin film on a substrate using focused ion beams. Micro-tensile tests are much more challenging because one has to machine “grips” on top of the micro-pillar so that a holder can grab the pillar and pull on it.

Using Molecular Dynamics and Dislocation Dynamics simulations, Wei Cai’s group has discovered a counter-intuitive behavior of dislocations in BCC pillars. When stress is applied to BCC pillars, dislocations do not simply exit the pillar (as they do for FCC pillars). Instead, the dislocations self-replicate and send other dislocation moving in the opposite direction before the first one exits the surface. This means that a single dislocation nucleation event in a BCC pillar can produce a larger amount of plastic deformation than for a corresponding FCC pillar.

It is very difficult to verify these simulation results directly from in situ experiments, but some research groups have started to design experiments that could ultimately test this prediction.

Reference

Surface Controlled Dislocation Multiplication in Metal Micro-Pillars. C.R. Weinberger and W. Cai, *Proceedings of the National Academy of Sciences*, 105, 14304–14307, 2008. doi:10.1073/pnas.0806118105

AHPCRC Tech Area 2 Research Team

Tech Area Lead: Eric Shaqfeh

Principal Investigators:

Dispersion of BWAs in Attack Zones

Mark Z. Jacobson
Civil and Environmental
Engineering Dept.,
Energy Resources Engineering
Dept.,
Director, Atmosphere/Energy
Program,
Stanford University
jacobson@stanford.edu
(650) 723-6836



Gianluca Iaccarino
Mechanical Engineering,
Stanford University
jops@stanford.edu
(650) 723-9599



and
Eric S. G. Shaqfeh
Chemical Engineering and
Mechanical Engineering Depts.,
Institute of Computational and
Mathematical Engineering,
Stanford University
esgs@stanford.edu
(650) 723-3764



Micro- and Nano-fluidic Devices for Sorting and Sensing BWAs & Engineering Blood Additives

Eric Shaqfeh

and
Eric Darve
Mechanical Engineering Dept.,
Institute for Computational and
Mathematical Engineering,
Stanford University
darve@stanford.edu.
(650) 725-2560



Molecular Dynamics Models of Antimicrobial Agents

Eric Darve

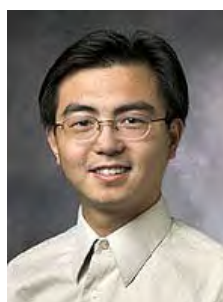
Protein Structure Prediction for Virus Particles

Jing He
formerly: Computer Science
Dept., New Mexico State
University
As of August 2009: Computer
Science Dept., Old Dominion
University
jhe@cs.odu.edu



Nano-Mechanics of Metal Plasticity in Thin Films and Cylinders

Wei Cai
Mechanical Engineering Dept.,
Stanford University
caiwei@stanford.edu
(650) 736-1671



AHPCRC Launches Summer Institute at Stanford University

The inaugural AHPCRC Undergraduate Summer Institute in Computational Science and Engineering was held at Stanford University from June 22 to August 14, 2009. Participants included 16 undergraduate students from five universities. Seventeen Stanford professors, research associates, postdocs, and graduate students served as instructors and mentors. This institute represents a key part of the AHPCRC mission: to foster the education of the next generation of scientists and engineers—including those from racially diverse and economically disadvantaged backgrounds—in the fundamental theories and best practices of simulation-based engineering sciences and high performance computing.

At this summer's institute, undergraduate students spent their mornings learning computational science and engineering concepts from experts in these fields. Several AHPCRC Stanford researchers offered instruction, including members of the research groups led by Charbel Farhat, Wei Cai, Eric Darve, and Pat Hanrahan. In addition, computer scientists from NVIDIA Corp. and AHPCRC consortium member High Performance Technologies, Inc. instructed the students in their own areas of expertise.

In the afternoons, students worked directly with AHPCRC researchers from groups led by Farhat, Darve, Cai, Hanrahan, and Leonidas Guibas. They simulated aircraft wings, submarines, bulletproof fabrics, and advanced nanoscale materials. They



taught camera networks to recognize and report their locations. And they helped to design the underlying computer algorithms and architectures that made the other projects possible. The students learned about numerical methods used in computational science and engineering, and they received an introduction to computational engineering methods and modeling, meshing computational domains, ordinary and partial differential equations, and optimization problems. They also learned to program in several commonly used computer languages and systems, including C, MATLAB, MPI, and specialized programming for GPU processors.

On August 14, the students presented the results of their research at a seminar, to which representatives from the U.S. Army were invited. Introductory remarks were given by Charbel Farhat, AHPCRC Director; Raju Namburu, Army Research Laboratory AHPCRC Cooperative Agreement Manager; and Barbara Bryan, AHPCRC Research and Outreach Manager. LTC Fredrick C. Ludden, Military Deputy, Army Research Laboratory Computational and Information Sciences Directorate, offered concluding remarks. ★



Above: Padilla, Ramirez, Gutierrez, DeVito.
Left: Chukwuka, Darve, Oriaifo
Right: Shaffer

Next page
Left: Murphy, Thompson
Right: Bou-Mosleh, Patel

Photos courtesy Barbara Bryan, HPTi





And the Results Are...

A list of students, mentors, and project titles appears on page 26. Below is an example of what the students and their mentors thought of their experience. Charbel Bou-Mosleh mentored Samir Patel on his project, “The Aerodynamic Analysis of a Damaged Wing.”

This was my first experience mentoring students in this type of setting. I spent most of my time with the two students I mentored, but I had some interaction with another student who was working on a different project. My students were getting their first experience with the methods and techniques we used. They worked on Linux workstations and clusters, using the commercial software MATLAB and Ansys ICEM [computational fluid dynamics meshing software], as well as Prof. Charbel Farhat’s research codes.

My students worked on projects that require “mesh generation.” This was a class they had to take 3 or 4 weeks after the summer school had started. If there was anything I would do differently, it would be to organize the classes so that students

could get earlier access to topics they were using in their projects.

The students worked very hard and they learned very fast. They almost finished what I had prepared for them a couple of weeks before their presentation day. Samir [Patel] in particular was working during the weekends. I was getting emails from him on Saturdays and Sundays at 7:00 PM sometimes. I thought that was impressive. In addition, Samir’s presentation skills were amazing. He’s very smart and has a good self-confidence.

— Charbel Bou-Mosleh, Stanford Engineering Research Associate, Department of Aeronautics and Astronautics

This program presented me with my first opportunity to do research in the field of aerodynamics. My experiences at Stanford have inspired me to explore the relationship of computational fluid dynamics to biology.

Everything I learned this summer was new knowledge! I was very happy with the setup of learning the theory in a classroom setting and then applying it using codes and other engineering software.

The purpose of my research was to use software to obtain results comparable to those obtained through physical testing of real models. The software I used included Ansys ICEMCFD, MATLAB, and a whole suite of software developed by Professor Farhat’s research group.

The instructors, especially my mentor Dr. Bou-Mosleh, were important in terms of teaching me the fundamentals of what I would be doing. Much of this took place in the morning sessions, when we spent a couple of hours learning about everything (and I emphasize, everything!). I collaborated with Dr. Bou-Mosleh since my project required me to understand new processes, software, and other CFD-related materials, and also troubleshoot various difficulties that arose throughout the research process. I will certainly keep in touch with everyone.

It seems as though engineering has taken a dramatic leap through supercomputing. It was amazing to run flight simulations without having to use a wind tunnel and a model wing.

— Samir Patel, undergraduate student, Harvard University

UTEP Summer Program Brings Computation to Life

The 2009 AHPCRC Education Program at the University of Texas at El Paso (UTEP) aims to increase the number of middle-school students capable of and interested in technical subjects by equipping middle-school teachers of mathematics and their students with appropriate motivating examples of the usefulness of mathematical concepts and by providing both the teachers and students with interactive computational technologies that can be used to refine associated mathematical knowledge and skills. In some cases different instances of an example are encapsulated in a computational tool, while in other cases the examples stand by themselves and can be, if desired, paired with computational tools.

The project was launched on 30 April 2009 by a visit from Dr. Robert M. Panoff, founder and Executive Director of Shodor, a non-profit education and research corporation dedicated to the reform and improvement of mathematics and science education by appropriate incorporation of computational and communication technologies. Our project uses the Shodor Web site as a main resource of computational tools, especially the hands-on, exploratory-learning tools associated with Project Interactivate (www.shodor.org/Interactivate).

A team of three undergraduate students (Victor Jordan Barraza, Fernando Nava, and Jason Shultes), one graduate student (Oscar Andrade), two faculty members (David Novick and Patricia Teller), and one research



staff member (Sarala Arunagiri) in the Department of Computer Science worked through the summer to develop a set of prototypes to motivate concepts related to probability and to refine the understanding and application of these concepts. The examples and associated computational tools that the team produced have been mapped to lessons and problems in the mathematics textbooks used by the El Paso Independent School District (EPISD) in the 6th, 7th, and 8th grades.

A Web site associated with the project will disseminate the project's products—the motivating examples and computational tools—as well as the mappings of examples and tools to textbook lessons and problems. Specific dissemination is aimed at middle-school teachers in EPISD, at faculty and staff who conduct outreach programs, and at AHPCRC partners. A section of the Web site will enable users of the examples and tools to provide feedback on the educational materials and their usefulness.

The project team worked with the staff of UTEP's Educational Talent Search (ETS) program—a TRIO



Photos courtesy Patricia Teller, UTEP.





program (see “*The Federal TRIO Programs*,” below) working with more than 600 low-income middle- and high-school youth in the El Paso area to provide information about college admission, careers, scholarships, financial aid and SAT/ACT preparation. ETS staff and the project team held a workshop for middle-school students on Monday, 10 August 2009, to get feedback on the prototypes developed to date. Eighteen 7th and 8th grade students from two schools participated. The ETS staff recruited the students (we developed brochures for this purpose), brought the students to campus, fed them breakfast, brought them to the workshop, and then took them to lunch, provided a campus tour in the form of a scavenger hunt, and returned them to the schools. In the workshop, the team’s undergraduate students presented some of the examples they developed, along with some of the computational tools they identified. The examples included:

- the “yield” of the iPod manufacturing process (i.e., the percentage of iPods produced that meet the specified standards of manufacture, which can be estimated by testing a sample set)—a study of sample spaces, probabilities, and algebra;
- the creation of an enhanced version of the paper, rock, scissors game—a study of probabilities and fairness; and
- the evolution of the solution of Rubik’s cube—a study of the number of possible permutations.

At the end of the workshop, each student was given a certificate of participation and a Rubik’s cube.

As part of the workshop, the middle-school participants provided feedback on the motivating examples and the tools that they tried out, and the project team

compiled simple descriptive statistics from their responses. The most popular computational tools were a simulation of fire in a forest using a grid populated with trees and a simulation of the population trends of a world of grass, rabbits, and foxes, again using a grid to implement the simulation. Preliminary review of the feedback and the reaction of the students and staff indicated that the project has an excellent chance of success!

The project’s next step, slated for this Fall, is a workshop for middle-school math teachers. This workshop is being designed to motivate the teachers to adopt the examples developed by the project and to develop examples of their own. In addition, the teachers will be encouraged to adopt the computational tools identified by the project, and to identify other computational tools that support their lesson plans. The workshop will give the teachers opportunities to provide the project team with feedback and to influence the direction of the project. During the Fall semester, the project’s undergraduate students will be available to work with the teachers and visit the schools to aid the teachers in the use of the teaching materials. ★

The Federal TRIO Programs for educational opportunity outreach are designed to motivate and support students from disadvantaged backgrounds. TRIO’s six outreach and support programs serve and assist low-income, first-generation college students and students with disabilities as they progress from middle school to postbaccalaureate programs. TRIO also includes a training program for directors and staff of TRIO projects. A dissemination partnership program encourages institutions and agencies that do not have TRIO grants to replicate or adapt successful practices of TRIO projects.

Source:
www.ed.gov/about/offices/list/ope/trio/index.html

AHPCRC Director Honored by U.S. Association of Computational Mechanics

Professor Charbel Farhat, AHPCRC program director, has received the 2009 John von Neumann Medal from the U.S. Association of Computational Mechanics (USACM) for “outstanding and sustained contributions in high performance computing, fluid–structure interaction, and computational acoustics and their impact on real-world engineering applications.”

Charbel Farhat, the Vivian Church Hoff Professor of Aircraft Structures and Chair of the Department of Aeronautics and Astronautics at Stanford University, was named director of the AHPCRC in 2007. He is internationally known for his outstanding research contributions to computational mechanics, numerical analysis, and high performance computing.

He has pioneered the development of parallel finite element solution methods that have enabled faster and more accurate analyses of a broad range of engineering and pathfinder systems such as re-entry vehicles, modern fighter aircraft, advanced Formula 1 cars, aircraft carriers, underwater systems, electronic packages, and nano-scale optical shutters. His achievements in this area have been recognized by several professional societies, including the IEEE Computer Society, which awarded him the Fernbach Award for “outstanding contributions to the development of parallel numerical algorithms and parallel software packages that have helped the mechanical engineering world to embrace parallel processing technology.”

His innovative theoretical and computational works on computational fluid dynamics on moving grids and fluid–structure interaction phenomena have contributed to a renaissance of research on nonlinear com-

Charbel Farhat,
Stanford
University photo.



putational aeroelasticity. These works have also had a profound impact on practitioners such as the flight test engineers at the Edwards Air Force Base, who stated that Farhat’s research has enabled them “to better simulate certain structural and aerodynamic flight qualities with the improved models.” They stated that this should allow them “to perform fewer flight tests and save time when we are flight testing.”

Computational Mechanics is concerned with the use of computational methods and devices to study events governed by the principles of mechanics. It is a fundamentally important part of computational science and engineering, concerned with the use of computational approaches to characterize, predict, and simulate physical events and engineering systems governed by the laws of mechanics.

The USACM is a prominent association that promotes U.S. research, commercial, and academic activities in the general area of computational mechanics. The John von Neumann Medal is the highest award it bestows to honor individuals who have made outstanding, sustained contributions in the field of computational mechanics, generally over periods representing substantial portions of their professional careers. The medal is awarded every two years at the time of the National Congress of the Association. ★

AHPCRC Website Offers News, Resources

<http://me.stanford.edu/research/centers/ahpcrc/index.html>



The AHPCRC website, hosted by Stanford University's Department of Mechanical Engineering, has information about all of the projects sponsored by this program. Visit the "Labs & Research" page for a directory of projects and researchers, as well as image archives for each of the four technical areas. The "Publications" page contains an up-to-date list of publications and presentations by AHPCRC researchers and all the back issues of the *AHPCRC Bulletin* in pdf format. "Education and Outreach" highlights the summer pre-college programs that are a part of the AHPCRC mission, and "News" keeps you current on honors and awards given to AHPCRC researchers and other items of interest. ★

AHPCRC Exhibit at Supercomputing 09

AHPCRC researchers and students from UTEP and NMSU, and HPTi staffers from Arlington, Stanford, and Dayton showed off the program's research efforts at Supercomputing 09, November 16–19, at the Oregon Convention Center in Portland, Oregon. Special thanks are due to the students from UTEP and NMSU who volunteered their time at the AHPCRC exhibit. For more conference information, see <http://sc09.supercomputing.org> ★



AHPCRC researchers, staff, and students at Supercomputing 09.
Photo by Jake Weyant, HPTi.

Publications and Presentations

AHPCRC Publications and Presentations January–June 2009

Project 1–1: Ballistic Impact and Optimization of Composite Shields

- Attachment mode performance of network-modeled ballistic fabric shielding. D. Powell, T. I. Zohdi. *Composites Part B: Engineering*, 40 (6), 451–460, September 2009, doi:10.1016/j.compositesb.2009.01.010.
- A note on flaw-induced integrity reduction of structural fabric. D. Powell, T. I. Zohdi. *The International Journal of Fracture/Letters in Micromechanics*, 158 (1), 89–96, July 2009. doi: 10.1007/s10704-009-9368-x.
- Microfibril-based estimates of the ballistic limit of multilayered fabric shielding. T. I. Zohdi. *The International Journal of Fracture/Letters in Micromechanics*, 158 (1), 81–88, July 2009. doi: 10.1007/s10704-009-9367-y.
- Multi-Scale Modeling and Large-Scale Transient Simulation of Ballistic Fabric. D. Powell, T. Zohdi, C. Farhat. 10th U.S. National Congress on Computational Mechanics, Columbus, OH, July 2009.
- Multi-Scale Modeling and Large-Scale Transient Simulation of Ballistic Fabric. C. Farhat, D. Powell, T. I. Zohdi. Presentation to Army Research Laboratory, Aberdeen Proving Ground, MD, April 2009.
- Modeling of Composite Materials at Multiple Scales. D. Arbelaez, T. I. Zohdi. Presentation to Army Research Laboratory, Aberdeen Proving Ground, MD, April 2009.

Project 1–4: Flapping and Twisting Aeroelastic Wings for Propulsion

- Numerical Study of Flexible Flapping Wing Propulsion. T. Yang, M. Wei, H. Zhao. Submitted to the 48th AIAA Aerospace Sciences Meeting, Orlando, FL, January 2010.
- Optimal Flight of Rufous Hummingbirds in Hover: An Experimental Investigation. H. B. Evans, J. J. Allen, B. J. Balakumar. Submitted to the 48th AIAA Aerospace Sciences Meeting, Orlando, FL, January 2010.
- Study of Flow Structures Around the Wing of a Scaled Robotic Hummingbird Model at a Range of Reynolds Numbers. H. B. Evans. Master's Thesis, New Mexico State University, 2009.
- Numerical Simulation of Flexible Flapping Wings in Fully-Coupled Motion. T. Yang, M. Wei, and H. Zhao. American Institute of Aeronautics and Astronautics (AIAA) Symposium, Las Cruces, NM, 2008.

Project 2–2: Micro- and Nano-fluidic Devices for Sorting and Sensing BWAs

- The Effect of Brownian Motion on the Stability of Sedimenting Suspensions of Polarizable Rods in an Electric Field. B. Hoffman, E.S.G. Shaqfeh. *J. Fluid Mech.* 624, 361–388 (2009).
- Simulation of Brownian, drug delivery particles in microchannel flows. A. Saibaba, E.S.G. Shaqfeh, E. Darve. Oral Presentation, 62nd Annual American Physical Society Division of Fluid Dynamics Meeting, Minneapolis, MN, Nov. 22–24, 2009.
- Numerical simulation of platelet margination in microcirculation. H. Zhao, E.S.G. Shaqfeh, E. Darve. Oral Presentation, 62nd Annual American Physical Society Division of Fluid Dynamics Meeting, Minneapolis, MN, Nov. 22–24, 2009.

Project 2–4 (was Project 2–3 for Years 1 and 2): Protein Structure Prediction for Virus Particles

- Structure Prediction for the Helix Skeletons Detected from the Low Resolution Protein Density Map. K. Al Nasr, J. He. Submitted to Asia Pacific Bioinformatics Conference, India, January 2010.
- Native Secondary Structure Topology has Near Minimum Contact Energy among All Possible Geometrically Constrained Topologies. W. Sun, J. He. *Proteins: Structure, Function and Bioinformatics*, 77 (1), 159–173, doi:10.1002/prot.22427, 2009.
- Characterization of Local Protein Structure Geometry from the Protein Data Bank—a Senior Project in Bioinformatics. J. Santini, B. Benson, J. He. *Proceedings of the Computing Alliance of Hispanic Serving Institutions Annual Meeting*, pp 49–51, Mountain View, CA, 2009.
- An Effective Convergence Independent Loop Closure Method using Forward-Backward Cyclic Coordinate Descent. K. Al Nasr, J. He. *International Journal of Data Mining in Bioinformatics*, 3 (3), 346–361, 2009, doi: 10.1504/IJDMB.2009.026712.
- Parallelized Simulated Annealing for Protein Topology Prediction. K. Al Nasr (presenter), W. Sun, J. He. Poster, Graduate Research and Arts Symposium, NMSU, April 22–23, 2009.
- Parallel Computing in Protein Structure Topology Determination. W. Sun, S. Al-Haj, J. He. *Proceedings of the 26th Army Science Conference*, CP8, Orlando, FL, December 2008.

Project 3–1: Information Aggregation and Diffusion in Networks

- Predictive QoS Routing to Mobile Sinks in Wireless Sensor Networks. B. Kusy, H.J. Lee, M. Wicke, N. Milosavljevic, L. Guibas. International Symposium on Information Processing in Sensor Networks (IPSN), April 2009.
- Dynamic Resource Management and Matching in Sensor Networks. J. Gao, L. Guibas, N. Milosavljevic, D. Zhou. International Symposium on Information Processing in Sensor Networks (IPSN), April 2009.

Distribution Statement A: Approved for public release; distribution is unlimited.

Publications and Presentations

- Lightweight Coloring and Desynchronization for Networks. A. Motkin, T. Roughgarden, P. Skraba, L. Guibas. *Proceedings of IEEE INFOCOM*, 2009.
- Interference-Aware MAC Protocol for Wireless Networks by a Game-Theoretic Approach. H.J. Lee, H. Kwon, A. Motkin, L. Guibas. *Proceedings of IEEE INFOCOM*, 2009.
- Exploiting Probabilistic Independence for Permutations. J. Huang, C. Guestrin, X. Jiang, L. Guibas. 12th Conference on Artificial Intelligence and Statistics (AISTATS), Clearwater Beach, FL, April 2009.

Project 3–2: Robust Wireless Communications in Complex Environments

- Robust Collaborative-Relay Beamforming. G. Zheng, K.-K. Wong, A. Paulraj, B. Ottersten. *IEEE Transactions on Signal Processing*, 57 (8), 3130–3143, 2009, doi: 10.1109/TSP.2009.2021456.
- Code Rate–Diversity–Multiplexing Tradeoff. E. Stauffer, D. Tujkovic, A. Paulraj. *IEEE Trans. Information Theory*, 55 (1), 245–254, 2009, doi: 10.1109/TIT.2008.2008127.

Project 3–3: Secure Sensor Data Dissemination and Aggregation

- Distributed jammer network: impact and characterization. H. Huang, A. Bhattacharya. Accepted for IEEE Milcom 2009, Boston MA, October 2009.

Project 4–2: Flexible Architecture Research Machine (FARM): Transactional Memory

- Presentation on the FARM system (title not available). O. A. Olukotun, C. Kozyrakis. Submitted to MICRO-42, the 42nd IEEE/ACM International Symposium on Microarchitecture, New York, NY, December 2009.

Project 4–3: Simulation & Modeling to Enhance the Performance of Systems of Multicore Processors

- On the Use of Shareable Resource Signature Characterization and Hardware Thread Priorities to Improve Simultaneous Multithreaded (SMT) Processor Throughput. M. R. Meswani, P. J. Teller, S. Arunagiri. Submitted to IEEE International Symposium on Workload Characterization (IISWC 2009), Austin, TX, October 2009.
- Supercomputing Research at NMSU: Processor Modeling for Large-Scale System Simulation. J. Cook. Presentation at the New Mexico State University Dean's Council Meeting at Intel, July 2009.
- Monte Carlo Processor Modeling of Contemporary Computer Architectures. J. Cook. Presentation at the Joint Operations Weapons Operations Group (JOWOG) meeting at Sandia National Laboratories, July 2009.
- Modeling and Analysis of Checkpoint I/O Operations. S. Arunagiri, J. T. Daly, P. J. Teller. *Proceedings of ASMTA 2009, the 16th International Conference on Analytical and Stochastic Modeling Techniques and Applications*, Madrid, Spain, June 9–12, 2009. Available from LNCS (Lecture Notes in Computer Science) 5513, pp. 386–400, doi: 10.1007/978-3-642-02205-0. (Download at <http://www.springerlink.com/content/h058551872nx>)
- Characterization of Microarchitectural Resource Utilization on Simultaneous Multithreaded (SMT) Processors using SMT Thread Signatures. M. R. Meswani, P. J. Teller, S. Arunagiri. Submitted to the 23rd International Conference on Supercomputing (ICS'09), Yorktown Heights, NY, June 2009.
- Computer Architectures and Supercomputing: Past, Present, and Future. J. Cook (recipient of the Bromilow Research Award for outstanding research in the College of Engineering at New Mexico State University). Bromilow Distinguished Lecture, March 2009.
- An I/O scheduling Algorithm for Storage Performance Virtualization. S. Arunagiri (poster presenter), Y. Kwok, P. J. Teller, S. Seelam. 10th LCI International Conference on High-Performance Clustered Computing (LCI'09), Boulder, CO, March 2009.
- Improved Throughput of Simultaneous Multithreaded (SMT) Processors using SMT Thread Signatures and Hardware Thread Priorities. M. R. Meswani (poster presenter) and P. J. Teller. 10th LCI International Conference on High-Performance Clustered Computing (LCI'09), Boulder, CO, March 2009.
- A Study of the Influence of the POWER5 Dynamic Resource Balancing Hardware on Optimal Hardware Thread Priorities. P. C. Trillo (paper and poster presenter), M. R. Meswani, P. J. Teller, S. Arunagiri. *Proceedings of the 2008 ITEA Live-Virtual-Constructive Conference*, El Paso, TX, Jan. 2009.
- Measuring and Validating Metrics used to Estimate Microarchitecture Resource Utilization: A Case Study of the IBM POWER5 Processor. M. R. Meswani (poster presenter), P. J. Teller, S. Arunagiri. *Proceedings of the 2008 ITEA Live-Virtual-Constructive Conference*, El Paso, TX, Jan. 2009.

Project 4–4: High Performance Optimization Library

- A Smoothing Algorithm for Solving QAPs. K.-M. Ng, W. Murray. 20th International Symposium on Mathematical Programming, Chicago, IL, August 2009.

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Publications and Presentations

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- Nonconservative Robust Control: Optimized and Constrained Sensitivity Functions. C.-M. Fransson, T. Wik, B. Lennartson, M. A. Saunders, P.-O. Gutman. *IEEE Trans. Contr. Sys. Tech.* 17 (2), 298–308, 2009.
- Stabilizing Policy Improvement for Large-Scale Infinite-Horizon Dynamic Programming. M. J. O'Sullivan, M. A. Saunders. *SIAM J. Mat. Anal. Appl.*, 31 (2), 434–459, 2009.
- An active-set convex QP solver based on regularized KKT systems. C. Maes and M. A. Saunders. Presented at BIRS Workshop 09w5101, Advances and Perspectives on Numerical Methods for Saddle Point Problems, Banff, Alberta, Canada, April 12–17, 2009. <http://www.stanford.edu/group/SOL/talks.html>
also: An Active-Set Convex QP Solver Based on Regularized KKT Systems. C.-M. Fransson, T. Wik, B. Lennartson, M. A. Saunders, P.-O. Gutman. *IEEE Trans. Contr. Sys. Tech.* 17 (2), 298–308, 2009.
- Compile-Time Symbolic Differentiation Using C++ Expression Templates. D. Kourounis, L. N. Gergidis, M. A. Saunders. *ACM Trans. Math. Softw.*, revised 27 Mar 2009, 28 pp.
- Decompositions of a rank-one corrected generator matrix of a Markov chain. M. Haythorpe (recipient, T. M. Cherry prize for best student presentation at ANZIAM 2009; paper will appear in the *ANZIAM Gazette*). Presented at Australian and New Zealand Industrial and Applied Mathematics (ANZIAM) 2009, Caloundra, Queensland, Australia, February 1–5, 2009.
- Optimality principles in nonequilibrium biochemical networks. R. M. T. Fleming, C. Maes, M. A. Saunders, Y. Ye, and B. O. Palsson. *Physical Review Letters*, submitted 6 February 2009, 4 pp.
- Fast Algorithms for Convex Constrained Multiobjective Optimization. V. Pereyra, J. Castillo, M. A. Saunders. *SIAM J. Scientific Computing*, submitted 21 Jan 2009, 15 pp.

Project 4–6: Hybrid Optimization Schemes for Parameter Estimation Problems

- Three posters (titles not available). C. Quintero, R. Sanchez, C. Ramirez. Society for the Advancement of Chicanos and Native Americans (SACNAS) UTEP Expo, University of Texas at El Paso, March 2009.
- Three posters (titles not available). C. Quintero, R. Sanchez, C. Ramirez. Affinity Research Group (ARG) Workshop, University of Texas at El Paso, February 2009.

Supplemental Task 1: Quality Software Process for Effective Large-Scale Software Development

- Software Process for Rapid Development of HPT Software Using CMake. W. Hoffman. 2009 DoD HPCMP Users Group Conference (UGC), San Diego, CA, June 2009.

Supplemental Task 6: Mobile Networking Institute Support

- Network Sciences Interdisciplinary Computing Environment (NiCE). J. Rentería. Naval Research Laboratory Emulation Workshop, February 2009.

Supplemental Task 7: Multiscale Reactive Modeling Institute Support

- An Investigation of KS-DFT Electron Densities used in Atoms-in-Molecules Studies of Energetic Molecules. A. D. Yau, E.F.C. Byrd, B. M. Rice. *J. Phys. Chem. A*, 113 (21), 6166–6171, 2009. doi: 10.1021/jp9010845.

AHPCRC Undergraduate Summer Institute in Computational Science and Engineering (Project title / Student(s) / Mentor(s))

- Flutter prediction for the F-16 Block 40 / Alex Sabatini (Stanford) / David Amsellem, Charbel Farhat
- Micro Air Vehicle Modeling / Ricardo Medina (NMSU), / Charbel Bou-Mosleh, Charbel Farhat
- The Aerodynamic Analysis of a Damaged Wing / Samir Patel (Harvard) / Charbel Bou-Mosleh, Charbel Farhat
- Higher Order Scattering on Submerged Objects / Kalesanmi Kalesanwo (Morgan State) / Paolo Massimi, Charbel Farhat
- Modeling Differing Structural Fabric Designs for Use in Ballistic Shields / Brandon Moultrie (Morgan State), Caraline Murphy (NMSU) / David Powell, Charbel Farhat
- Sparse Matrix Solvers for Multi-Core and Parallel Platforms / Emilio Lopez and Andres Morales (Stanford) / Cris Cecka, Eric Darve
- Automated Calibration of Camera Networks / Daniel Shaffer (Stanford) / Branislav Kusy, Martin Wicke, Leonidas Guibas
- Full Cache Coherency on an FPGA-based Accelerator / Kevin Thompson (NMSU) / Sungpack Hong, Kunle Olukotun
- Mesh Visualization Tool / Richard Gutierrez (NMSU), Edgar Padilla and Essau Ramirez (UTEP) / Zach Devito, Pat Hanrahan, Eric Darve
- Characterization of High-Strength Nano-scale Gold and Aluminum / Michael Hammersley (Stanford) / Chris Weinberger, Sylvie Aubry, Wei Cai
- Thermal Conductivity of GaN Nanowires / Abraham Chukwuka (Morgan State) / Sylvie Aubry, Wei Cai
- Highly Anisotropic Iron in Fusion and Nuclear Power Plants / Stacey Oriaifo (Morgan State) / Sylvie Aubry, Wei Cai ★



AHPCRC Consortium Members

Stanford University
High Performance Technologies, Inc.
Morgan State University
New Mexico State University at Las Cruces
University of Texas at El Paso
NASA Ames Research Center



c/o High Performance Technologies, Inc.
11955 Freedom Drive, Suite 1100
Reston, VA 20190-5673
ahpcrc@hpti.com
703-682-5368

<http://me.stanford.edu/research/centers/ahpcrc>

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TECHNOLOGY DRIVEN. WARFIGHTER FOCUSED.

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